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Effect of (Ag, Sn) Doping on the Structure and Optical Properties of Au Nanocluster RADHAKRISHNAN BALU, SHASHI KARNA, US Army Rsch Lab - Aberdeen — Noble metal nanoclusters (NCs) consisting of a few to 35 atoms in size in the sub 2 nm range dimension are considered to be nontoxic as opposed to nanoparticles that are cytotoxic. Also, due to the quantum confinement of electrons, these NCs exhibit atom-like energy spectrum and display fluorescent properties useful in a wide range of applications, including medical diagnosis. The unique features of NCs such as size-tunable optical properties, intense fluorescence in the visible, and biocompatibility have stimulated an active area of investigation of noble metal NCs comprised of Au, Ag, Cu, and Pt. Furthermore, the electronic properties of nanoclusters can be modified by combining them with other elements. In this study, we consider the space-filled configuration of Au₃₂ NC and investigate the effects of Ag and Sn atom incorporation on geometry and electronic spectrum. Our study suggests that Ag and Sn doping of Au₃₂ NC red-shifts the absorption maximum and also reduces the oscillator strength.

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